Parcours Intelligence Artificielle

Machine Learning for Network Modeling

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Why are we here?

Short course on **Machine Learning** for **Network** Modeling

Planning: 4 dense sessions, 2.5 hours each

1. Introduction to Graph Theory and Network Science
2. Network models - Static and dynamic graphs*
3. Structure and topology inference
4. Processes and signals over graphs

* Session 2 is going to be given by Fabian Tarissan, CNRS, ENS Paris-Saclay

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How we’ll get through this?

Attend the courses

Do a short project

- It can be something around using the tools of the course for a problem of your main discipline or a thematic you’d like to pursue in the future
- The subject and perimeter of each project should be discussed
- Deliverables: report + codes (Matlab, R, Python, …)

.:: In this lecture

1. How to define structure when studying networks
2. Why network ‘structure’ matters
3. Community detection
4. Possible projects

Structure in Network Science

Structure in networks

- Macro-level:
  - Degree distribution
  - Small-world phenomena (i.e. short diameter)
  - # Connected components
  - Network model
- Meso-level:
  - Motifs (e.g. triads, cliques, cores, …)
  - Group behavior (for dynamic graphs)
  - Structural holes / weak ties
  - Community structure
- Micro-level:

  Node-user modeling
  - Static: reciprocity, node’s relation to communities: hub, internal, interface nodes, …
  - Dynamic: Actions (for dynamic graphs)

Distant cousins

Link analysis … qualitative

Network analysis … quantitative

Recall: Direct vertex connectivity

non-connected

simply connected

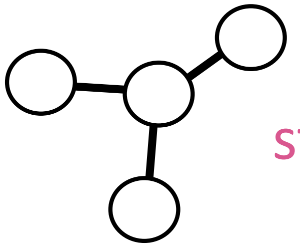
one-way connected

two-way connected
(*reciprocity*)

Meso: Graph motifs

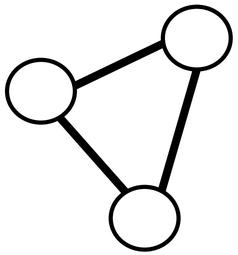
Graph motifs are statistically significant sub-graphs or patterns existing in a graph

- Very complicated to work with large motifs
- Usual analysis goes up to motifs of 3 to 5 nodes



star motif

Clique is a complete (sub)graph of vertices that is totally connected (i.e. complete) – … *restrictive*!!



clique

<u>Clique relaxations</u>

k-clique is a set of vertices among any pair of which the distance (shortest path) < k

k-club (or k-plex) is a set of vertices that has diameter < k

Clique relaxation: the paths can pass from anywhere in the graph, not just the induced subgraph

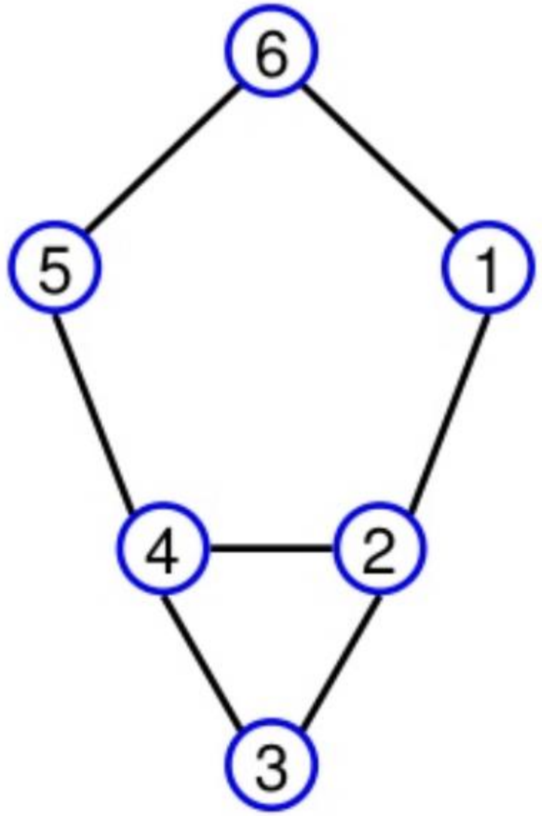
Meso: Graph motifs

Examples

- {2,3,4} is a 1-club (also regular clique)
- {1,2,4,5,6} is a 2-club
- {1,2,3,4,5} is a 2-clique but <u>not</u> a 2-club

(Note: Ain this case we consider the 5 vertices as part of the full graph amd therefore 1 is 2 hops away from 5)

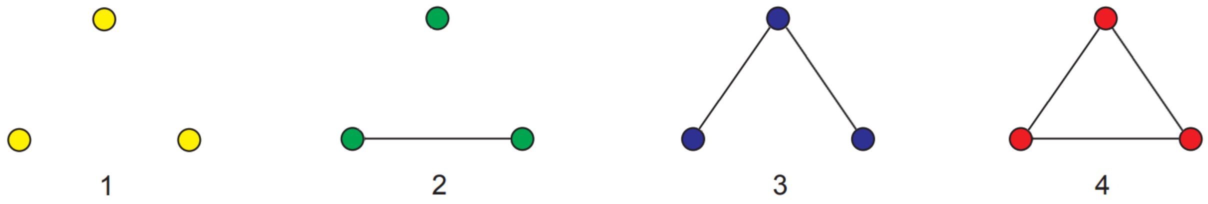
Clique relaxation: the paths can pass from anywhere in the graph, not just the induced subgraph



Meso: Graph motifs

The 4 possible undirected triads

Triads are motifs that can be formed between three vertices



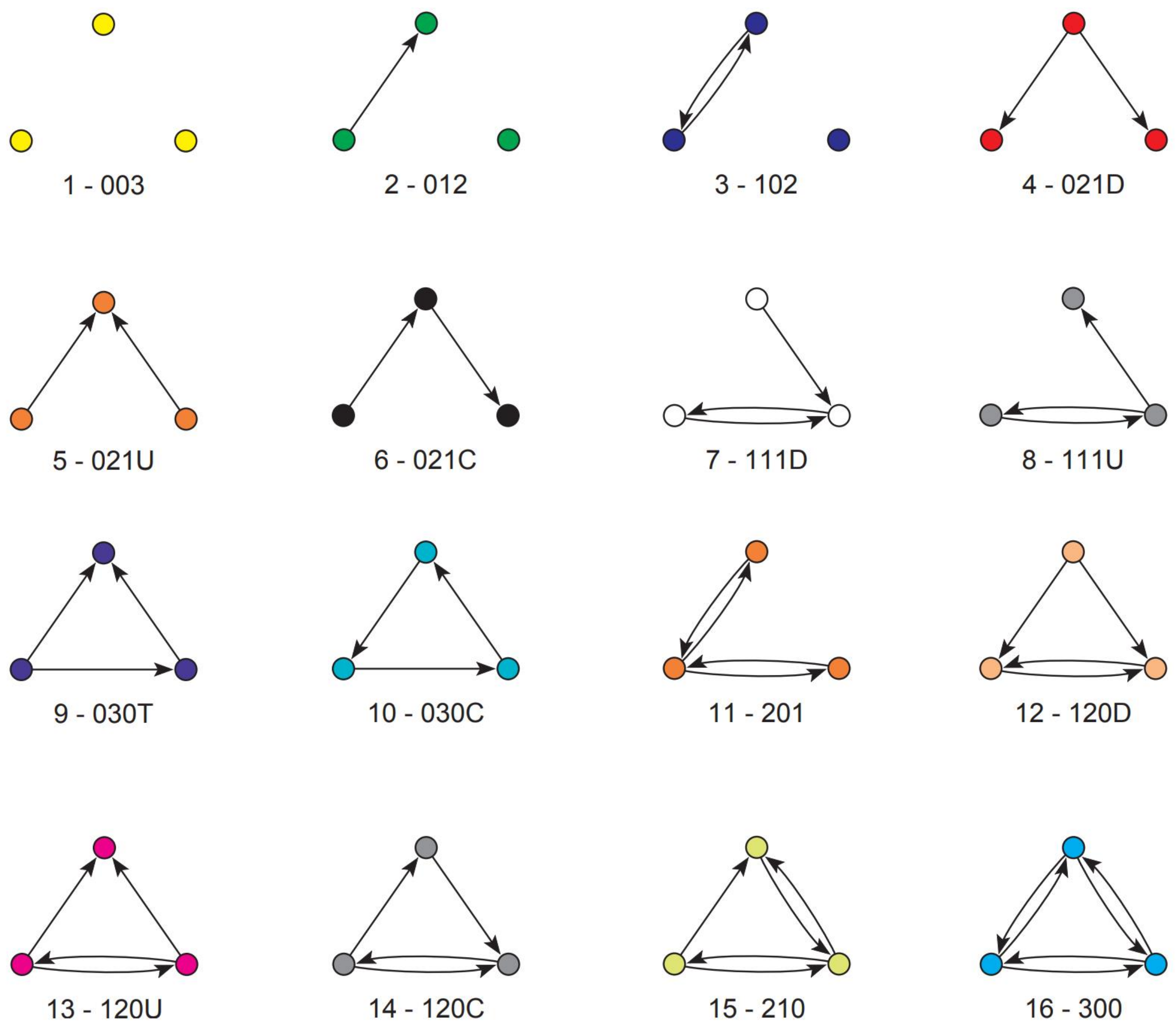
Also a clique

Labeling undirected triads can done using the numbering 1…4

- $label - 1$ = # edges in triad

Meso: Graph motifs

The 16 possible directed triads



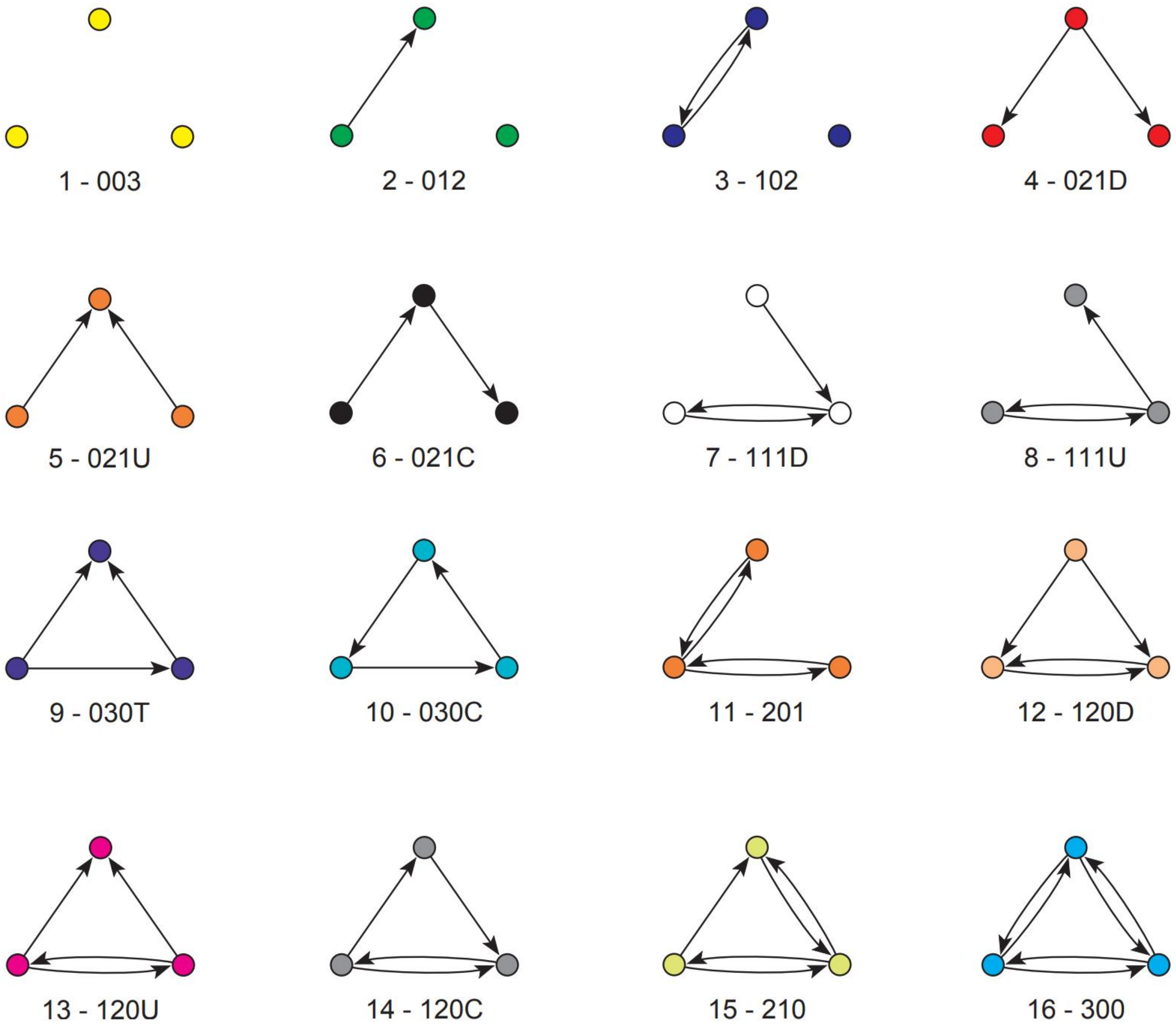
Labeling undirected triads can be done

- either by the numbering 1…16
- or by using a format *xyz*
  - *x* – # pairs of vertices connected with bidirected edges
  - *y* – # pairs of vertices connected with one-direction edges
  - *z* – # non-connected pairs of vertices
  - When unclear, use also one letter:

  Down, **U**p, **C**yclic, **T**ransitive

Meso: Graph motifs

The 16 possible directed triads



Transitivity in triads

If there are edges $u \rightarrow v$ and $v \rightarrow w$, then there exists also the edge $u \rightarrow w$

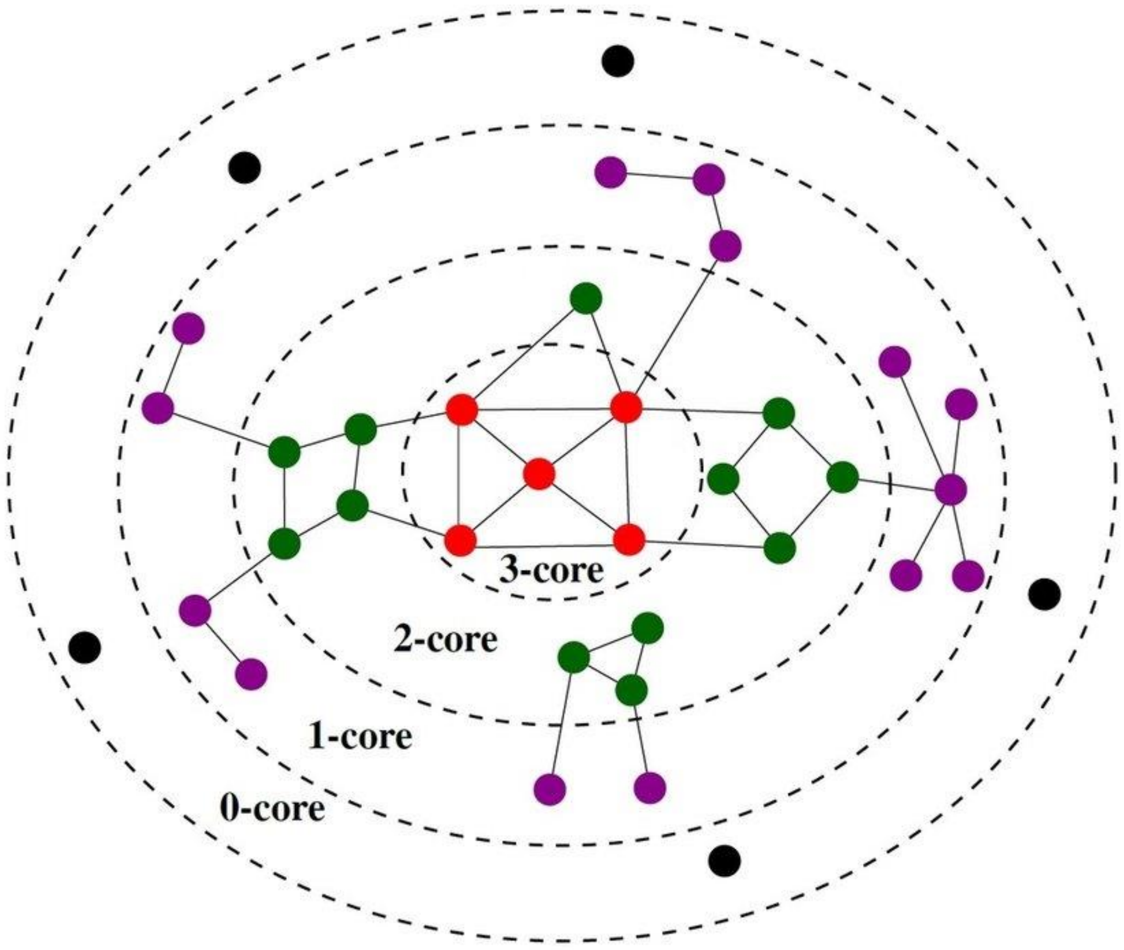
Labeling undirected triads can be done

- Triads 9, 12, 13, 16 are transitive
- Triads 6, 7, 8, 10, 11, 14, 15 are intransitive (… to different levels)
- Triads 1, 2, 3, 4, 5 are vacuously transitive (i.e. cannot be categorized)

Meso: Graph cores

A k-core is a maximal connected (sub)graph, whose vertices have at least degree k (to vertices that belong or not to the core)

- Cores do not respect density!!



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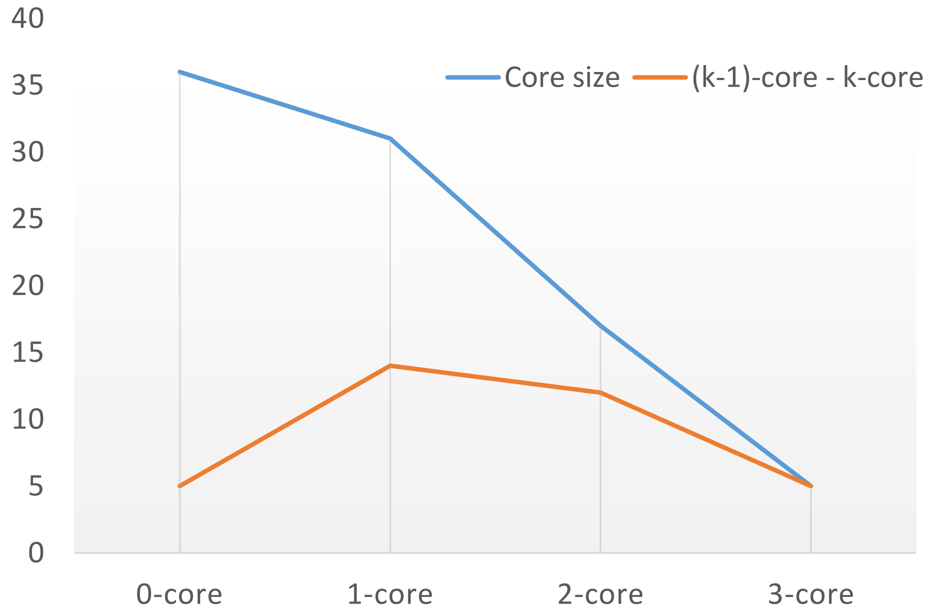
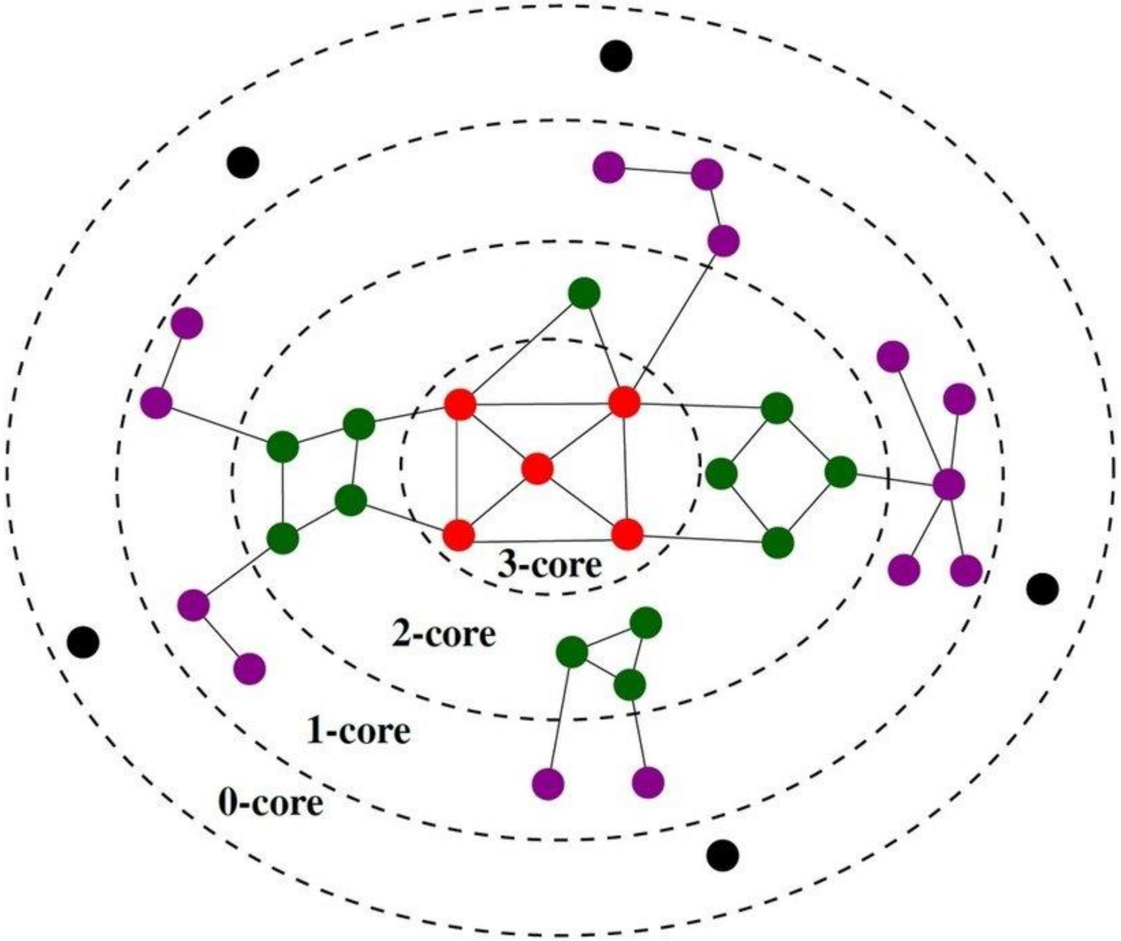
Graph degeneracy analysis





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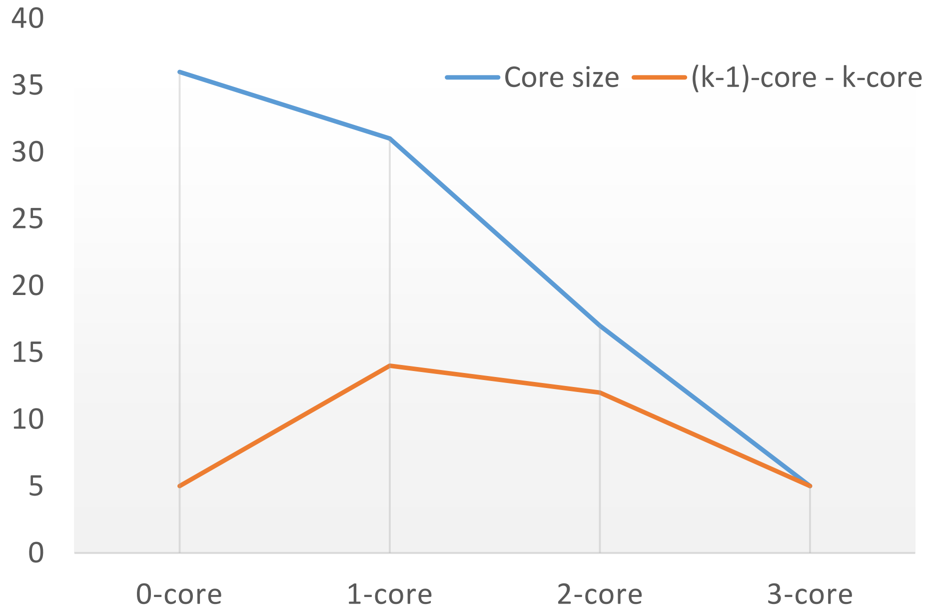
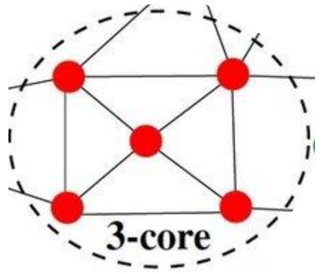
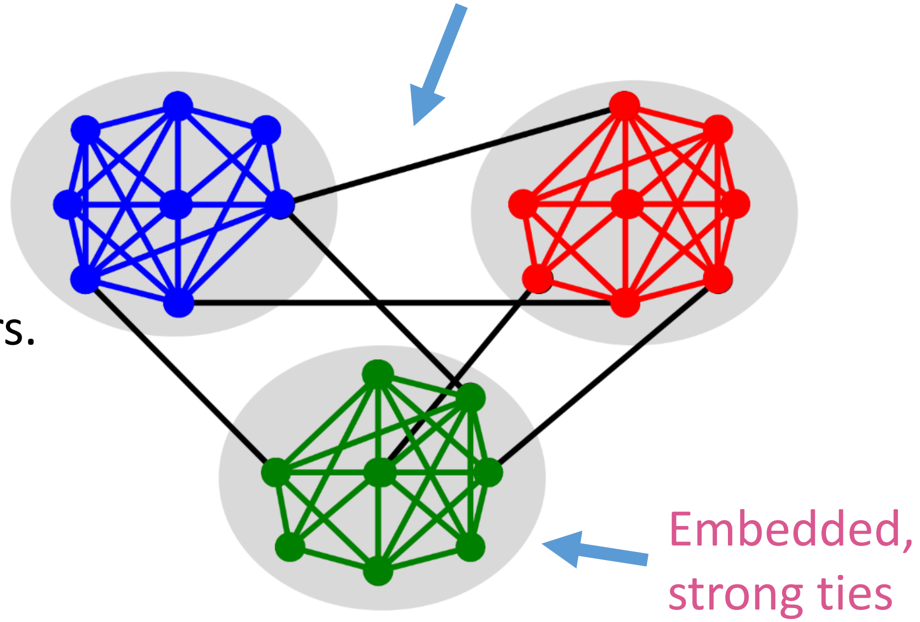




Also a 2-clique and a 2-club

Meso: Density/clusters/communities



Clusterability (Statistical ML principle)

Intra-cluster density / inter-cluster density $\gg 1$

Network closure

Homogeneity is higher inside a cluster than across different clusters.
New edges are more likely to appear inside clusters.

Triadic closure

Emergent edges will most likely `close' some triangle

Weak-ties property

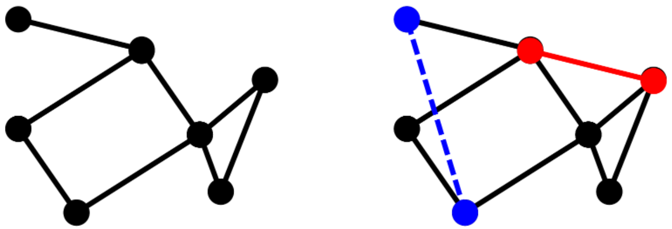
The strongest the connection (tie) between two individuals, the more likely they share contacts. Weak-ties are responsible for most communication among clusters.

Structural hole

(Similar to the above but with the opposite direction of causality)

Is the gap between two individuals who have complementary sources to information.

Triadic closure



Network cohesion

- The concept of network cohesion is central for answering many questions:
- Definitions depend on the context
  - Scale from **local** (e.g. triads) to **global** (e.g. giant component)
  - **Explicit** (e.g. cliques) or **implicit** (e.g. clusters) definition
- Desirable in-group properties of any **cohesive group:**
  - *Familiarity*… high degree
  - *Reachability*… small distance
  - *Robustness*… conectivity
  - *Density*… edge density
- Cliques indeed maximize these properties but… are restrictive!
  - Large cliques are super rare
  - They are sensitive: one edge destroys the property
  - Usually very costly to identify, or find maximal cliques in a graph (NP-complete)

Network cohesion - Density

- Global network density: measures how close to being a clique

$$density(G) = \frac{N_e}{N_v(N_v - 1)/2} \in [0,1]$$

This is for the whole undirected graph, but can be applied also to subgraphs

- Alternatively, it can be seen as a rescaling of the average degree

$$\bar{d}(G) = \frac{1}{N_v} \sum_{v \in V} d_v = \frac{1}{N_v} 2N_e \xRightarrow{repl.\, N_e} density(G) = \frac{\bar{d}(G)}{N_v - 1}$$

- Local density at node v: we can use the v's egonet, i.e. the subgraph induced by its neighbors

Network cohesion – Clustering coefficient

- Clustering coefficient of node v: measures the fraction of v's neighbors that are connected (here E_v is the #edges in the v's egonet)

$$cl(v) = \frac{2E_v}{d_v(d_v - 1)} \in [0,1]$$

- Global (average) clustering coefficient

$$cl(G) = \frac{1}{N_v} \sum_{v \in V} cl(v)$$

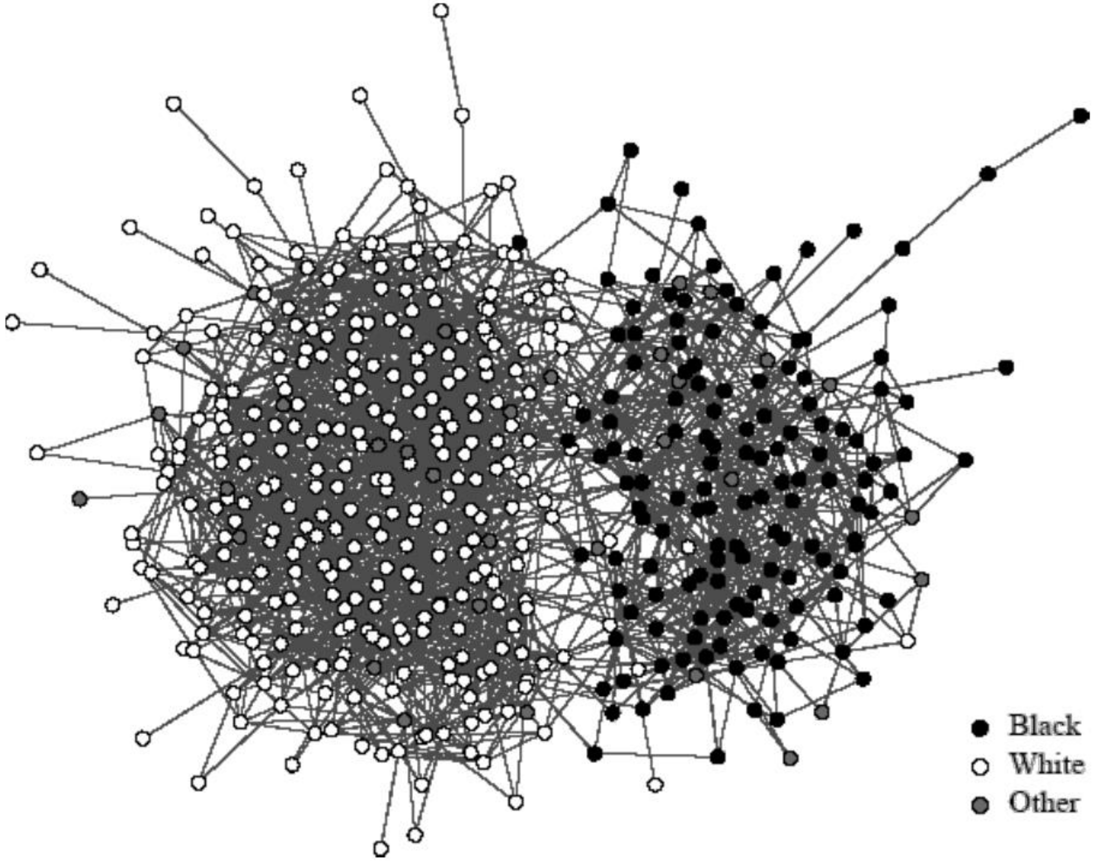
Assortative mixing

- Homophily or assortative mixing

  Individuals tend to get connected/interact with equal/similar others
- **Example**: high-school students by race, bloggers by political party, …
- Assortativity coefficient

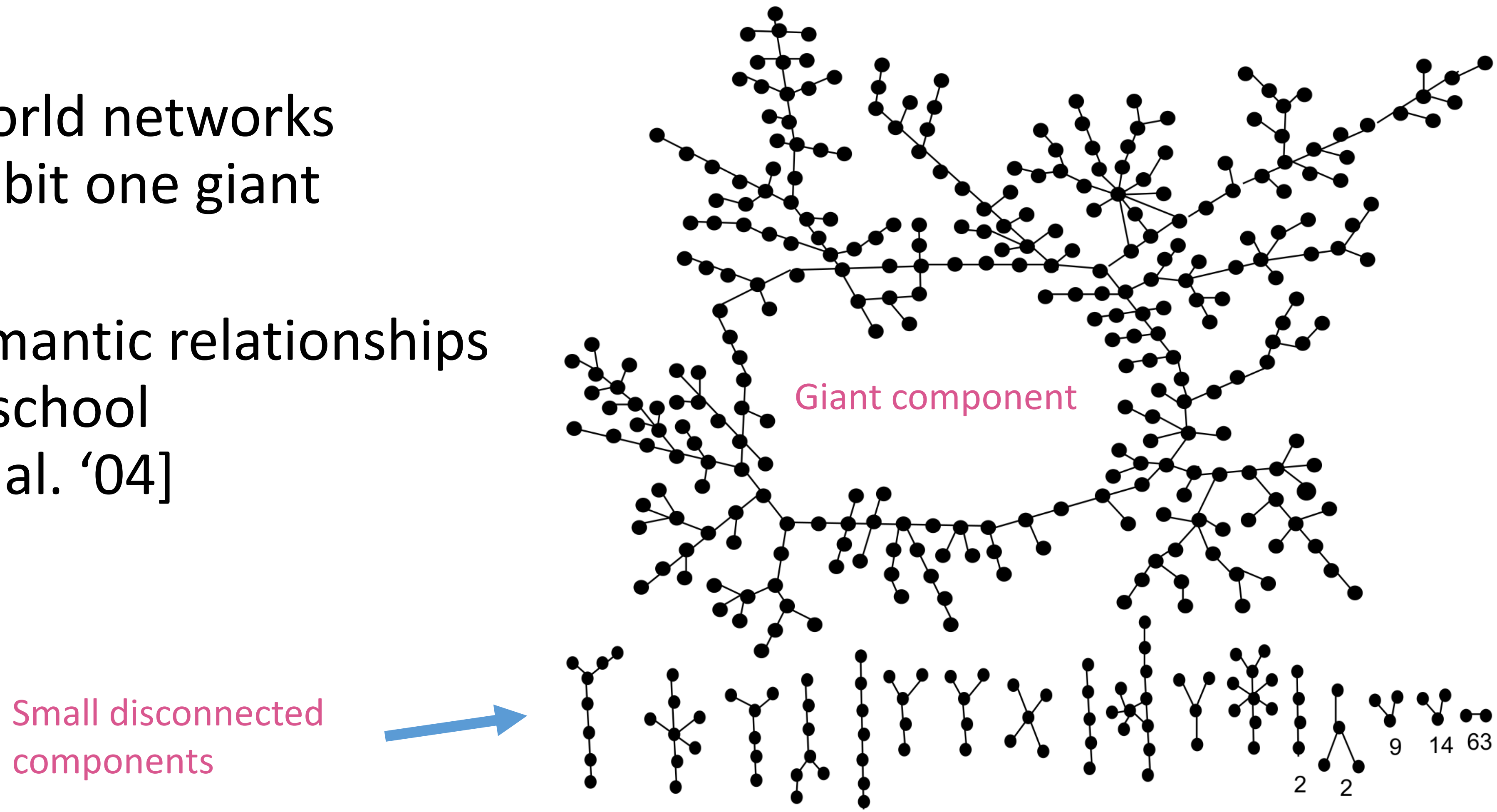
  Measures this property [Newman ’03]
- Dissasortative mixing exists too…

  e.g. romantic relationships between *males* and *females*

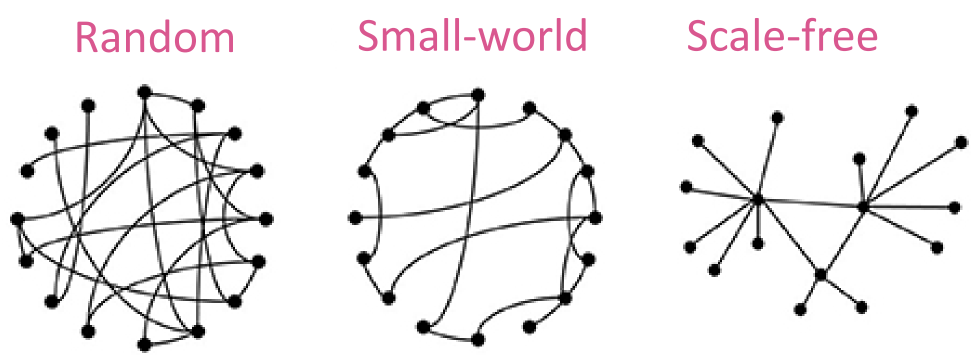


Network cohesion – Giant component

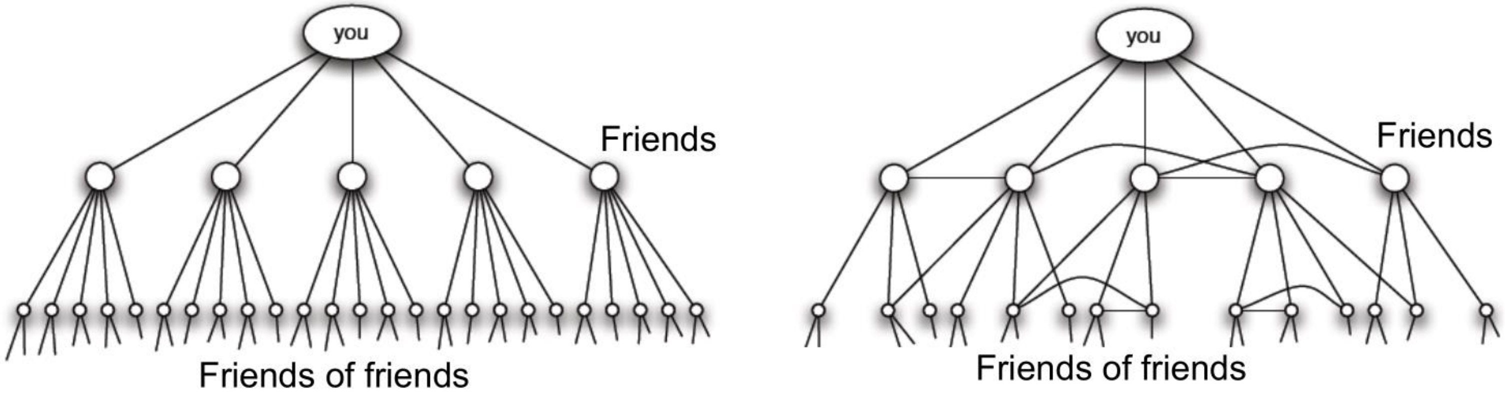
- Large real-world networks typically exhibit one giant component
- **Example**: romantic relationships in a US high school [Bearman et al. '04]



Small world phenomenon



- It refers to small average (shortest) path length $\approx O(\log Nv)$
- Intuitively… long hops reduce drastically the length of paths

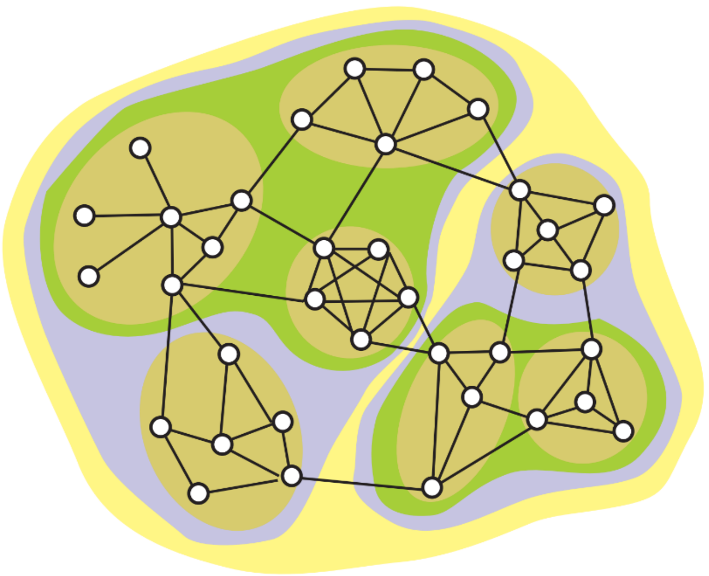


- This property facilitates the spread of information, diseases, etc…
- **Put in perspective**: Spread speeds-up in one cluster, yet a different cluster may be the reason to get 'blocked'

Network cohesion – Group centrality

- Recall node centrality measures
  - ***Closeness centrality***: the node has small average shortest path to other nodes
  - ***Betweeness centrality***: the node is frequently part of the shortest path between pairs of other nodes
- These can be extended to measure group centrality

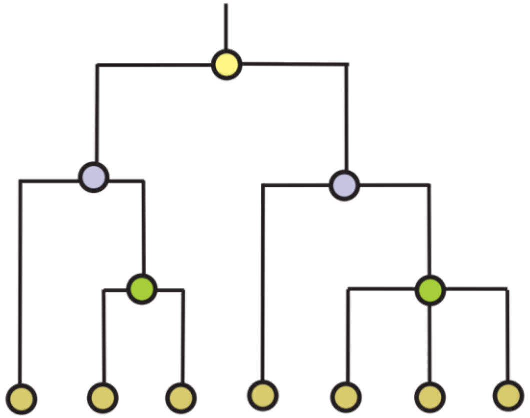
Global vs local graph views



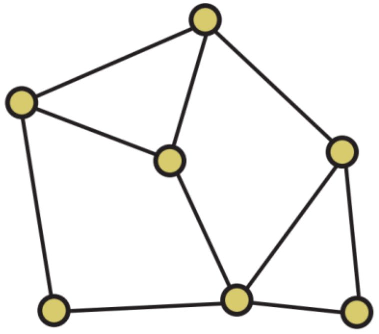
Global views

Local views

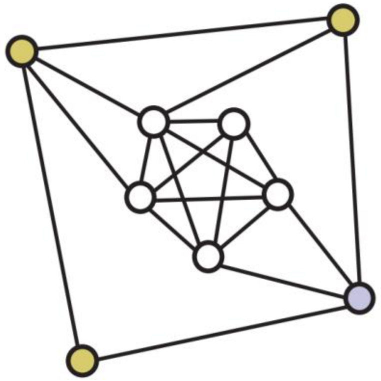
Hierarchical



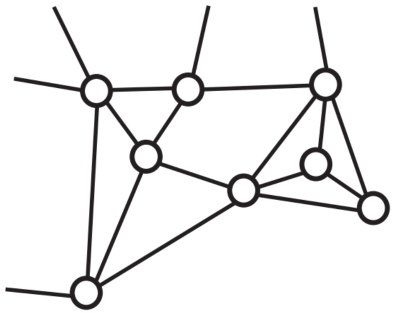
Reduction



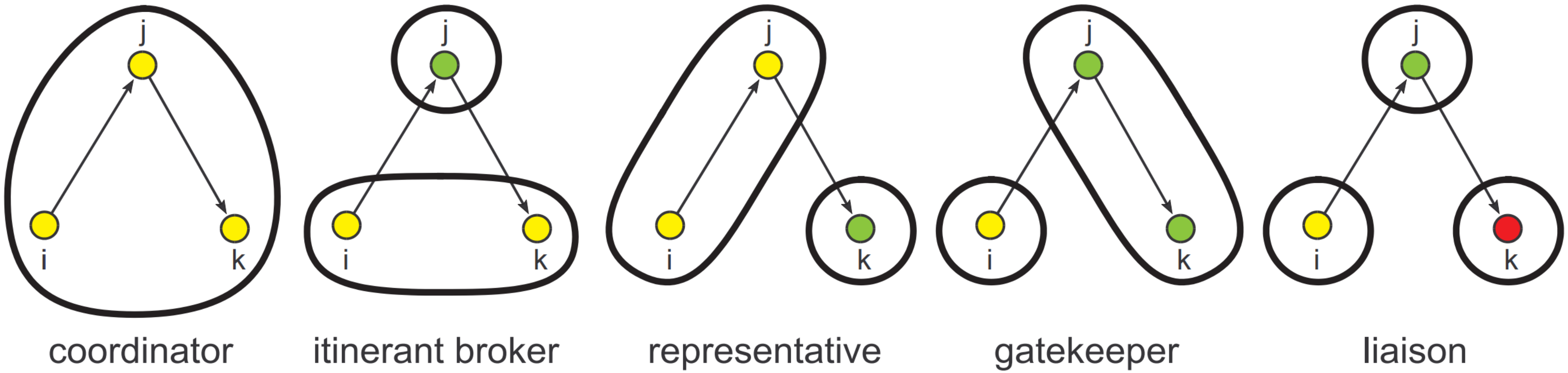
Context



Cluster cut-out

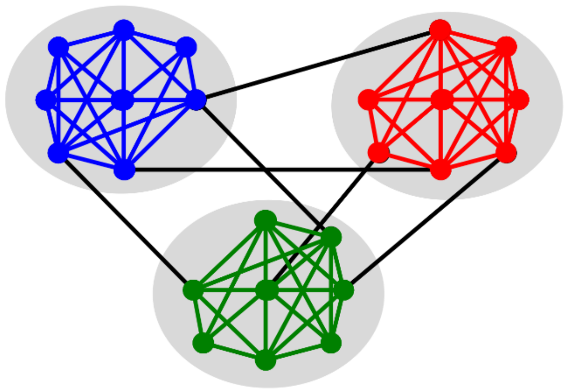


Micro: Node ‘roles’



Community detection

Community detection

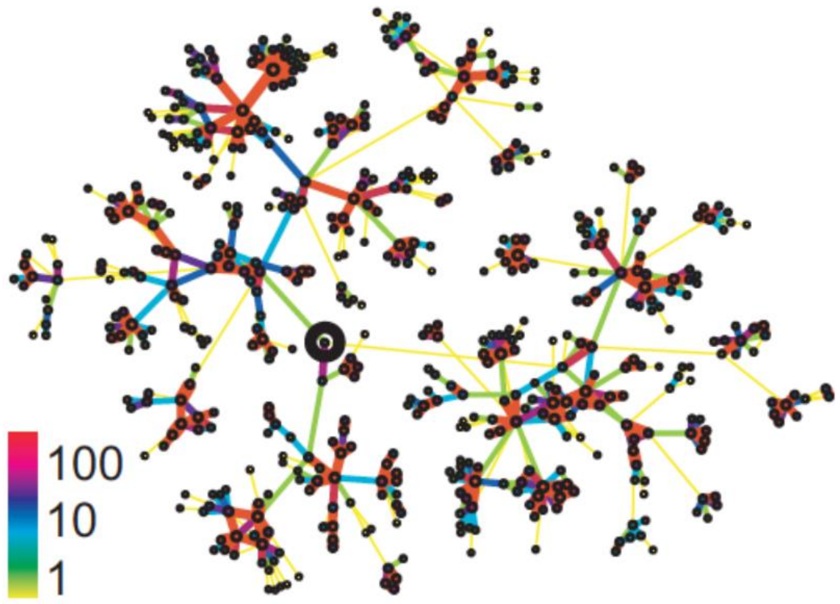


Split V into a given number k (non-overlapping) groups

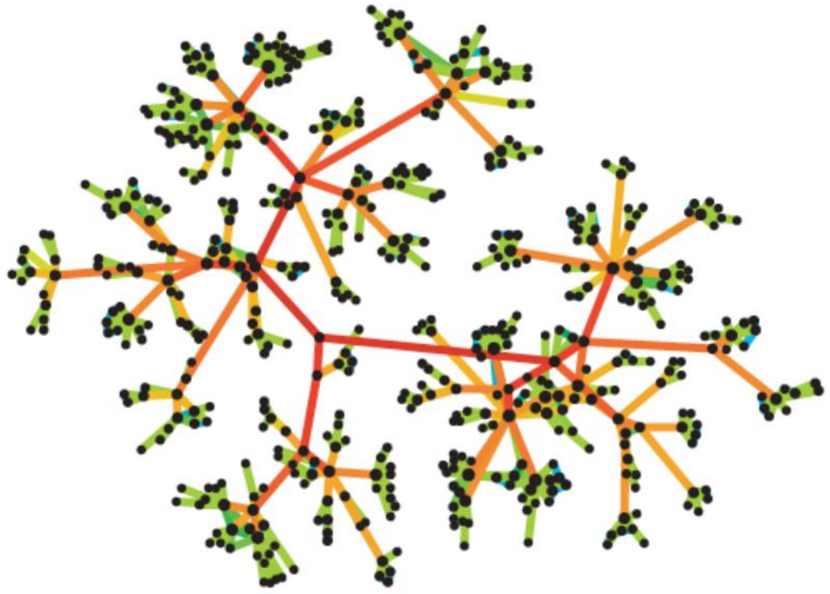
- Finding communities in networks is a challenging clustering problem
  - No concensus on the definition of « *what is a cluster* »
  - NP-hard problem: i.e. there are combinatorics behind separating optimally subsets of vertices and the problem cannot be solved in polynomial time.
  - Lack of ground truth to validate results
- Result of great interest for a plethora of reasons
  - Understanding data
  - Visualization
  - Compression
  - …

Graph partitioning

- Idea: try removing local bridges (weak ties) to decompose the graph
  - Combinatorial problem again: these may be many and with different importance
- Idea: target edges with large edge betweeness centrality (eBC)
  - These edges are part of many shortest paths among vertices
  - => stand at the interface between clusters



Edge strength



Edge betweenness

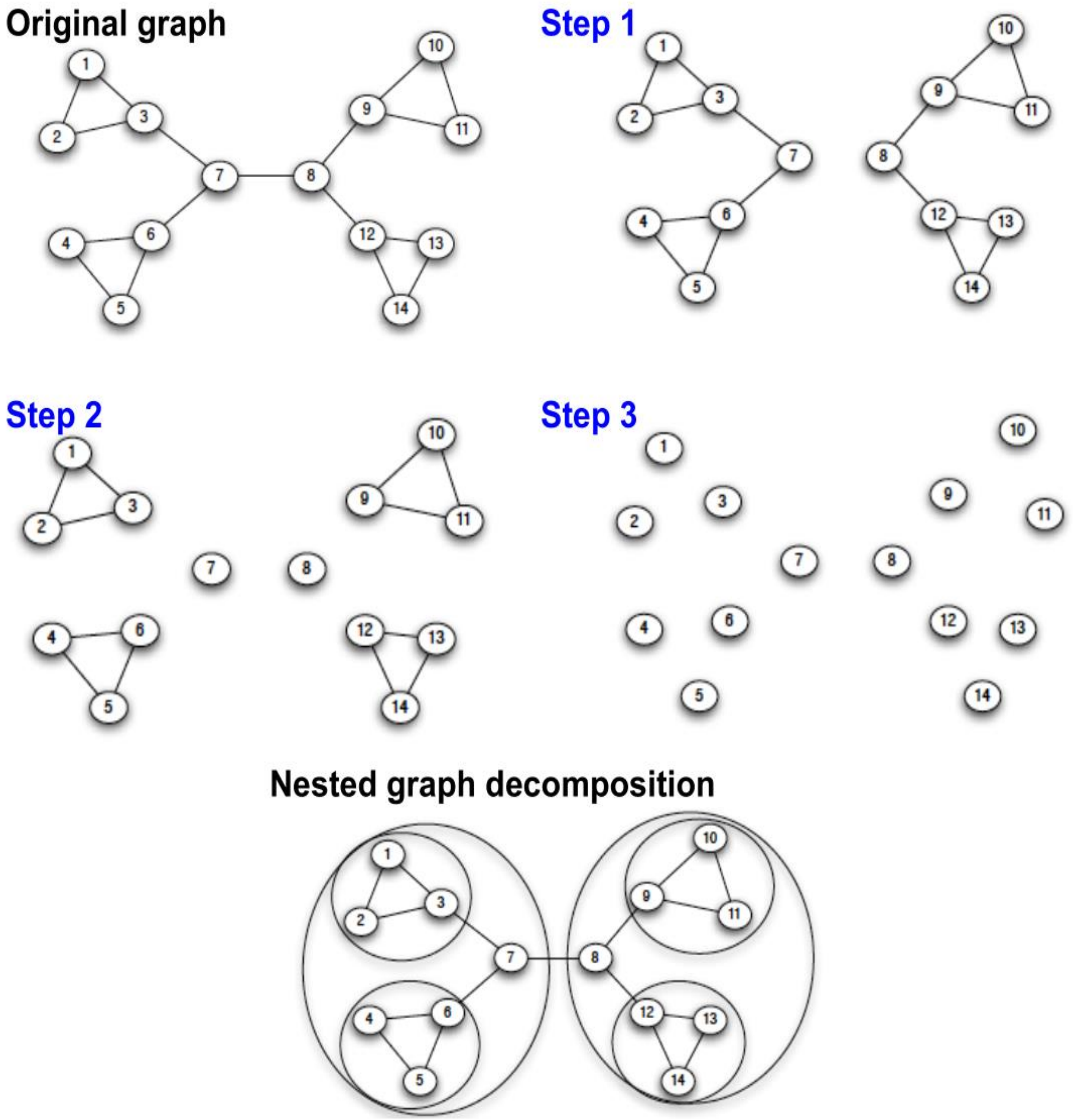
Girvan-Newman’s method

- Idea: Find and remove spanning links between cohesive subgroups
- **Algorithm**: Repeat until there are no edges left
  - Calculate the eBC of all remaining edges
  - Remove the edges(s) with the highest eBC
- What we get
  - Different connected components as communities
  - Nested partitioning (top-down), returns a dendrogram
  - Requires recomputing all centralities at each step $O(N_v N_e)$

M. Girvan and M. Newman, “Community structure in social and biological networks,” PNAS, 2002

Girvan-Newman's method

In action



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Hierarchical clustering

- A greedy approach that successively changes the solution
  - Agglomerative: is merging groups (bottom up)
  - Divisive: is splitting groups
  - Returns a *dendrogram* with all the hierarchical structure
  - Cutting the hierarchy at any level γ (from the top) gives $\gamma + 1$ clusters
- At each step the change should minimize a cost function
  - This measures the dissimilarity between the vertices in each group
  - Many options; a simple one is just the Euclidean or Manhattan

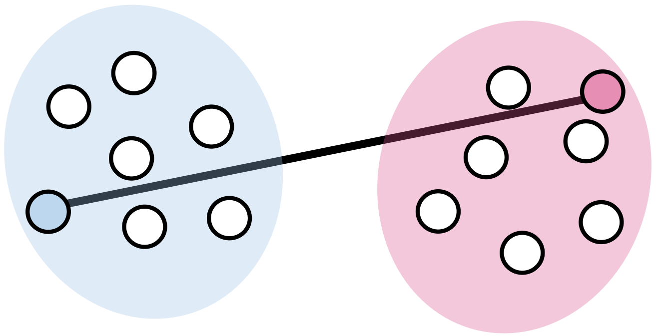
Agglomerative clustering

- Hierarchical Agglomerative clustering (bottom up)
  - 1) Choose dissimilarity metric between groups (!!)
  - 2) Assign each vertex to its own singleton group (1 vertex per group)
  - 3) Merge the two groups with the smallest dissimilarity
  - 4) Compute the dissimilarity of the new group with the preexisting ones
  - 5) If the current number of groups > 1 … **goto** (3)

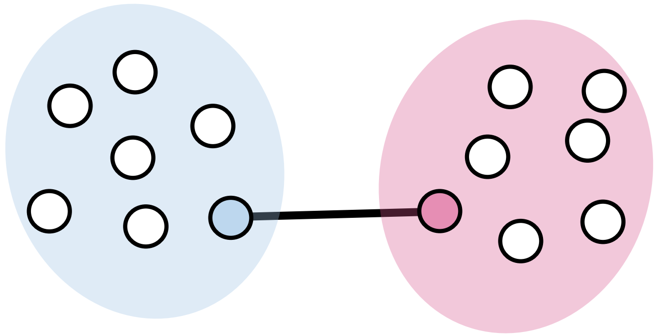
- Most critical part is to define group similarity

Agglomerative clustering

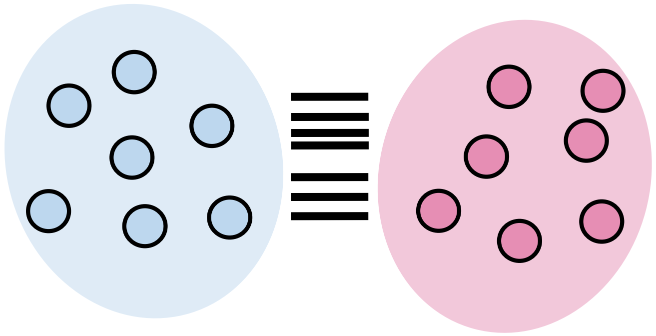
Single linkage



Complete linkage

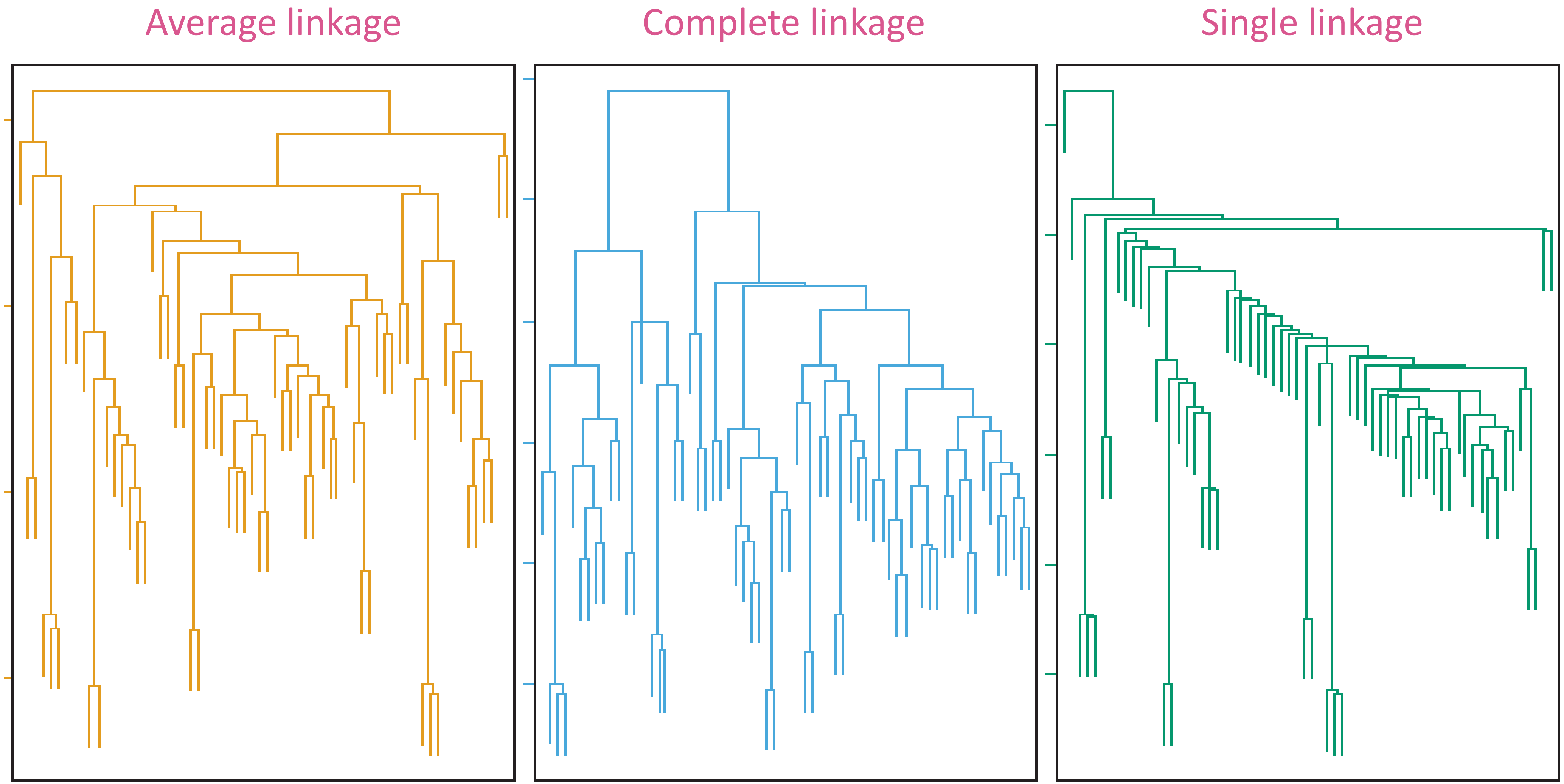


Average linkage



Agglomerative clustering

In action – dendrograms



Modularity-based community detection

Modularity

- Consider a graph G and a partition into groups $s \in S$

$$Q(G,S) \propto \sum_{s \in S} [(\#\text{ of edges within group } s) - \mathbb{E}\,[\#\text{ of such edges}]]$$

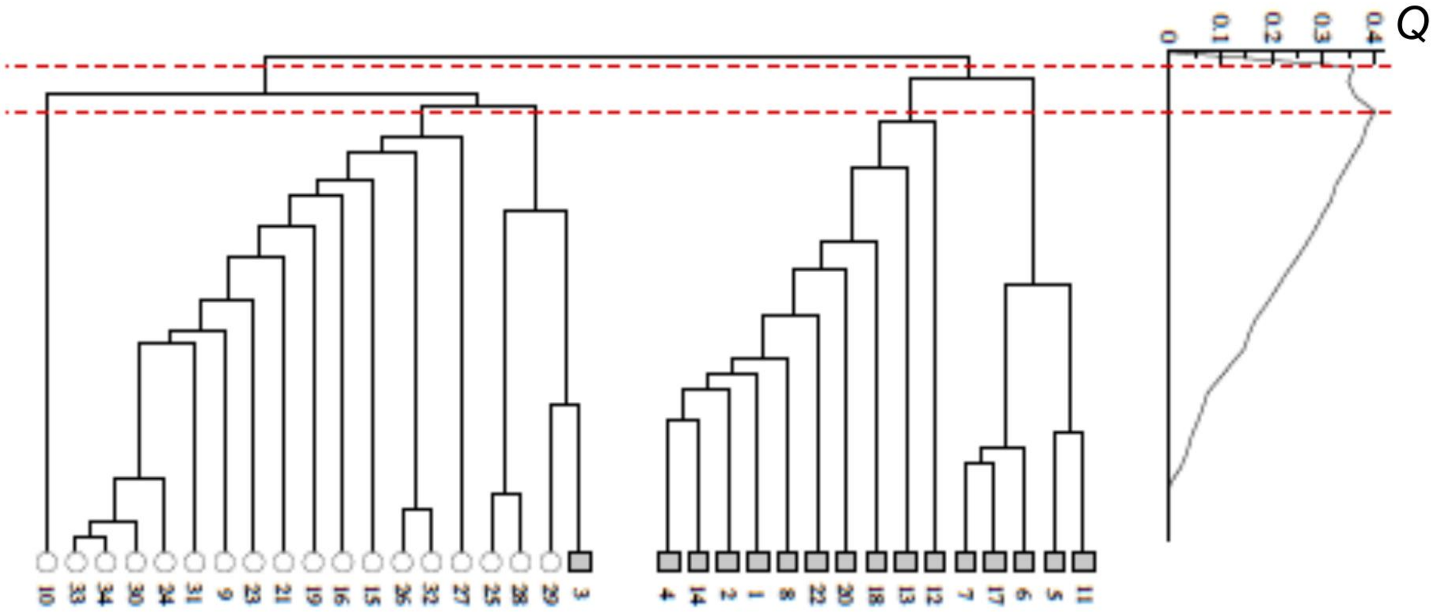
- After normalization such that $Q(G,S) \in [-1,1]$

$$Q(G,S) = \frac{1}{2N_e} \sum_{s \in S} \sum_{i,j \in s} \left[A_{ij} - \frac{d_i d_j}{2N_e} \right]$$

- *Null model*: one with random edges that preserves the degree distribution!

Modularity-based community detection

- We can evaluate modularity at the levels of a hierarchical dendrogram
- Keep the solution of the level that gives the ‘best’ community structure w.r.t Q



- Why not to optimize the partitioning directly w.r.t Q

Modularity-based community detection

Optimizing modularity

- Define a modularity matrix B with entries $B_{ij} = A_{ij} - \frac{d_i d_j}{2Ne}$
- Any *2-partition* S can be defined by a {+1,-1} binary vector $s = [s_1, \dots, s_{N_v}]^\mathrm{T}$
- Modularity gets a quadratic form

$$Q(G,S) = \frac{1}{4N_e} \sum_{i,j \in V} B_{ij} s_i s_j = \frac{1}{4N_e} \mathbf{s}^\top \mathbf{B} \mathbf{s}$$

- For **graph bisection** (2-split) the modularity-based criterion is formulated as

$$\hat{\mathbf{s}} = \arg \max_{\mathbf{s} \in \{\pm 1\}^{N_v}} \mathbf{s}^\top \mathbf{B} \mathbf{s}$$

- Due to the ‘nasty’ binary constraints of s makes this optimization is NP-hard!

Modularity-based community detection

The relaxation of constraints yields a feasible optimization

- By letting constraints $s \in \mathrm{R}^{N_v}$, $||s||_2 = 1$ we get

$$\hat{\mathbf{s}} = \arg\max_{\mathbf{s}} \mathbf{s}^\top \mathbf{B}\mathbf{s}, \quad \text{s. to} \;\; \mathbf{s}^\top \mathbf{s} = 1$$

- Associate a Langrange multiplier λ to the constraint $\mathbf{s}^\top \mathbf{s} = 1$
- Optimality conditions yields

$$\nabla_{\mathbf{s}} \left[\mathbf{s}^\top \mathbf{B}\mathbf{s} + \lambda(1 - \mathbf{s}^\top \mathbf{s}) \right] = \mathbf{0} \Rightarrow \mathbf{B}\mathbf{s} = \lambda \mathbf{s}$$

- Conclusion: s is an eigenvector of B with eigenvalue λ
- At the optimum $Bs = \lambda s$ the objective becomes

$$\mathbf{s}^\top \mathbf{B}\mathbf{s} = \lambda \mathbf{s}^\top \mathbf{s} = \lambda$$

To maximize modularity, pick the dominant eigenvector of B

Modularity-based community detection

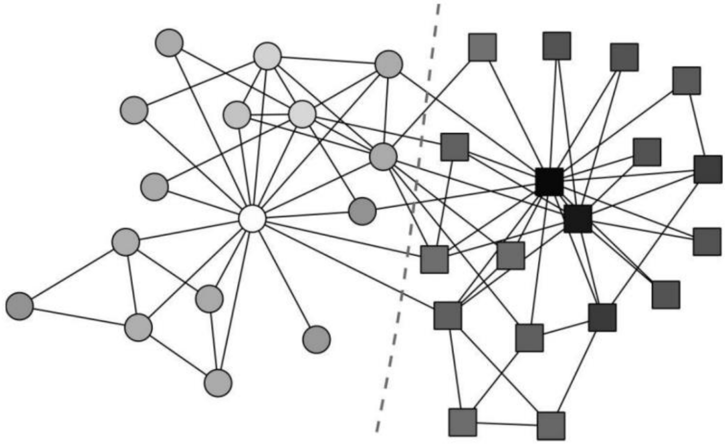
- Spectral modularity maximization algorithm

  S1: Compute modularity matrix $\mathbf{B}$ with entries $B_{ij} = A_{ij} - \frac{d_i d_j}{2N_e}$

  S2: Find dominant eigenvector $\mathbf{u}_1$ of $\mathbf{B}$ (e.g., power method)

  S3: Cluster membership of vertex i is $s_i = \text{sign}([\mathbf{u}_1]_i)$

- Multiple (> 2) communities through e.g., repeated graph bisection



Zachary's karate club

Spectral clustering

One moment… lets recall some spectral properties of the matrix representations of a graph

Graph Laplacian

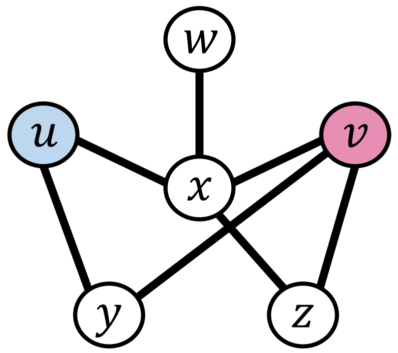
Although there are many definitions for Laplacian matrix, the most common is the following N_v x N_v

$$L = D - A$$

where D is a matrix with the degrees of the graph vertices in its diagonal, and zero values everywhere else

Graph Laplacian

Graph



Laplacian matrix L

	u	v	w	x	y	z
u	2			-1	-1	
v		3		-1	-1	-1
w			1	-1		
x	-1	-1	-1	4		-1
y	-1	-1			2	
z		-1		-1		2

=

Degree matrix D

	u	v	w	x	y	z
u	2					
v		3				
w			1			
x				4		
y					2	
z						2

−

Adjacency matrix A

	u	v	w	x	y	z
u				1	1	
v				1	1	1
w				1		
x	1	1	1			1
y	1	1				
z		1		1		

Graph Laplacian

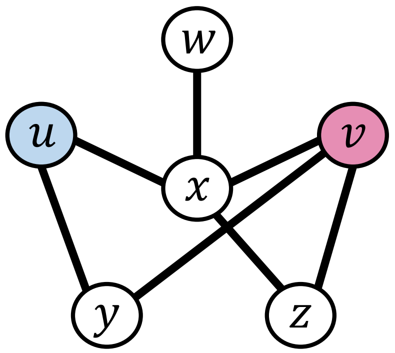
Basic properties

- Zero-sum rows and columns ==> zero-sum matrix L
- All negative values except in the diagonal
- Same off-diagonal zeros as A has information only for the directly connected pairs of vertices
- The input graph G cannot be a multigraph, edge weights are ignored
- Like in multivariate calculus, for (a problem-specific) $x \in \mathrm{R}^{N_v}$ that comes from some function $f(G, \ldots)$,

$$x^{\mathrm{T}} L x = \sum_{(i,j) \in E} (x_i - x_j)^2 = \sum_{i,j \in [1,\ldots,N_v]} A_{ij} (x_i - x_j)^2$$

The closest $x^{\mathrm{T}} L x$ is to zero, the more smooth the x is with respect to the graph, and so for the f

Graph



Laplacian matrix L

	u	v	w	x	y	z
u	**2**			**-1**	**-1**	
v		**3**		**-1**	**-1**	**-1**
w			**1**	**-1**		
x	**-1**	**-1**	**-1**	**4**		**-1**
y	**-1**	**-1**			**2**	
z		**-1**		**-1**		**2**

Eigen-analysis of graph Laplacian

Generally, L's eigenvalues and eigenvectors yield a lot of interesting information for a graph regarding

- G's connectivity
  - The smallest eigenvalue is 0 with eigenvector **1**
  - If the second smallest eigenvalue is 0 then the graph is disconnected. The multiplicity of 0's gives the # of components
  - The larger the non-trivial eigenvalues, the more connected a graph is
  - A connected graph of diameter δ has at least $\delta + 1$ distinct eigenvalues

- G's conductance (how fast does a random walk converge)
- the potential growth of a diffusion on G
- …

Graph Laplacian

Alternative definition: the normalized Laplacian matrix

$$\tilde{L} = D^{-\frac{1}{2}}\, L\, D^{-\frac{1}{2}}$$

$$= D^{-\frac{1}{2}}\,(D - A)D^{-\frac{1}{2}} = (D^{-\frac{1}{2}}D - D^{-\frac{1}{2}}A)\, D^{-\frac{1}{2}}$$

$$= D^{-\frac{1}{2}}DD^{-\frac{1}{2}} - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = I\; - D^{-\frac{1}{2}}\, A\, D^{-\frac{1}{2}}$$

Properties

- Symmetric, positive semi-definite with n non-negative eigenvalues
- The smallest eigenvalue is 0 with eigenvector $D^{-1/2}\mathbf{1}$
- More appropriate when there is degree inhomogeneity
- Constraints the eigenvalues in [0, 2]

Spectral clustering

Principle

1. Use the spectral property of $\mathbf{L}$ to perform clustering in the eigen space
2. If the network have K connected components, the first K eigenvectors are $\mathbf{1}$ span the eigenspace associated with eigenvalue 0
3. Applying a simple clustering algorithm to the rows of the K first eigenvectors separate the components

$\rightsquigarrow$ This principle generalizes to a graph with a single component: spectral clustering tends to separates groups of nodes which are highly connected together

Spectral clustering

Algorithm

Input: Adjacency matrix and number of classes Q

Compute the normalized graph Laplacian $\mathbf{L}$
Compute the eigen vectors of $\mathbf{L}$ associated with the Q smallest eigenvalues
Define $\mathbf{U}$, the $p \times Q$ matrix that encompasses these Q vectors
Define $\tilde{\mathbf{U}}$, the row-wise normalized version of $\mathbf{U}$: $\tilde{u}_{ij} = \frac{u_{ij}}{\|\mathbf{U}_i\|_2}$
Apply k-means to $(\tilde{\mathbf{U}}_i)_{i=1,\dots,p}$

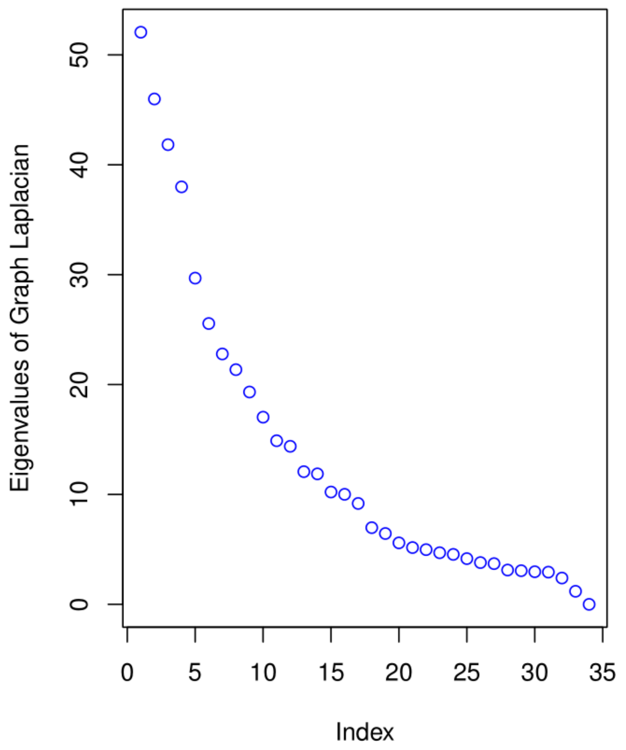
Output: vector of classes $\mathbf{C} \in \mathcal{Q}^p$, such as $C_i = q$ if $i \in q$

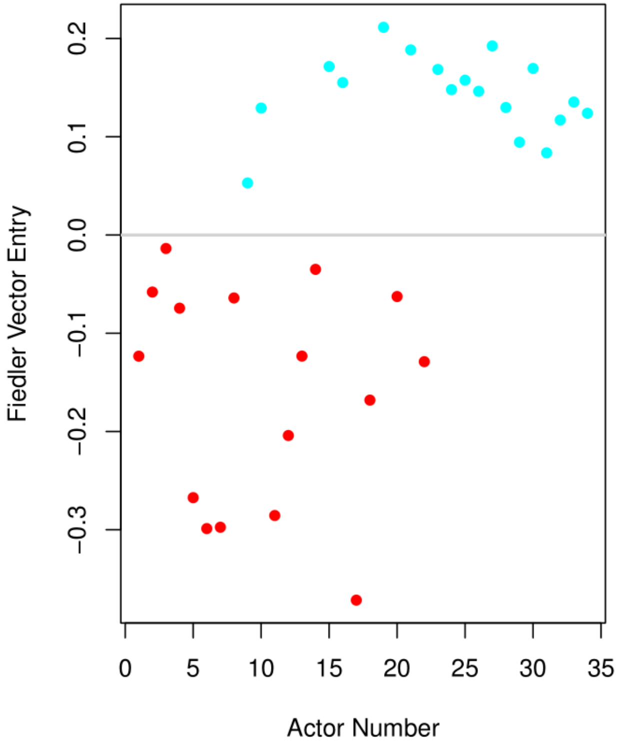
Algorithm 2: Spectral Clustering by Ng, Jordan and Weiss (2002)

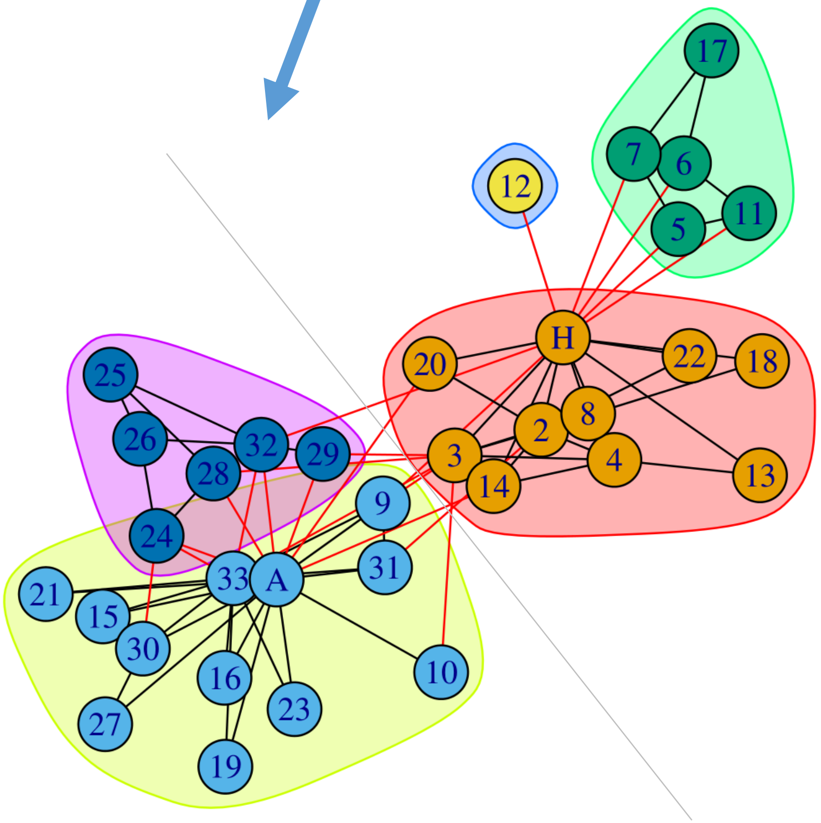
Spectral clustering

Split decided according to the **Fiedler vector**: the eigenvector corresp. to the **2nd smallest eigenvalue**

Example on Zachary's karate club







Possible projects

Possible projects @ Centre Borelli

- Graph degeneracy and traversals
  - *Density-Friendly Graph Decomposition* (Tatti 2019)
- Community detection
  - *The Inclusion Measure for Community Evaluation and Detection in Unweighted Networks* (Koufos&Likas 2018)
- Linear graph arrangement algorithms
  - Using various methods, e.g. *multigrid framework* (Safro et al)
- Graph signal processing
  - *Graph signal processing for machine learning: A review and new perspectives* (Dong, Thanou et al. 2020)
- Stability of ecological networks (survey)
  - *Complexity and stability of ecological networks: a review of the theory* (Landi et al. 2018)
  - *Unveiling dimensions of stability in complex ecological networks* (Dominguez-Garcia et al. 2019)

Discussion

Q & A